Lecture 2
The Hamiltonian approach to classical mechanics.
Analysis of vibrations in one-dimensional lattice.

Program:
1. Vibrations of a simple diatomic molecule.
2. Lattice vibrations in a monoatomic 1D lattice: modes and dispersion relations.

Questions you should be able to answer by the end of today's lecture:
1. The Hamiltonian analysis of vibrations in a 1D monoatomic lattice?
2. The graphical representation of solutions – dispersion relations.
3. What is the physical significance of the shape of the dispersion relations?

References:
1. Kittel, Chapter 4, page 99.
2. Ashcroft and Mermin, Chapter 22, page 422.

Example III: 1D Diatomic molecule

Here we will consider a simple diatomic molecule – let's say H2, where two hydrogen atoms are bound to each other with a single sigma bond. Since the bond is stretchable and compressible to a certain extent we can approximate it with a spring, and approximate the hydrogen atoms as balls attached to its ends. We will soon learn that this model doesn't work to explain electronic structure but for our purposes of understanding lattice vibration it provides a sufficient framework.

I. The system: Two atoms (approximated) by balls of mass *m* are bound by a stretchable bond approximated with a spring of length *l* and stiffness *K*. Here the position and momentum of the left atom are x_1 and p_1, the position and momentum of the right atom are x_2, p_2.
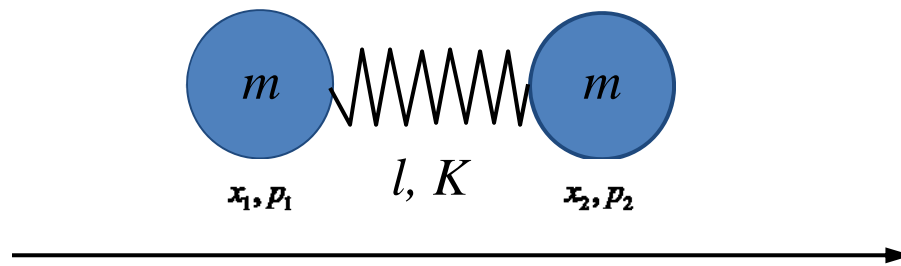
II. The Hamiltonian.

The energy for this molecule is: $E = \dfrac{mv_1^2}{2} + \dfrac{mv_2^2}{2} + K\dfrac{\Delta l^2}{2} = \dfrac{p_1^2}{2m} + \dfrac{p_2^2}{2m} + \dfrac{K}{2}\left(x_2 - x_1 - l\right)^2$

Then the Hamiltonian for this system is:

$$H\left(x_1, p_1; x_2, p_2\right) = \dfrac{p_1^2}{2m} + \dfrac{p_2^2}{2m} + \dfrac{K}{2}\left(x_2 - x_1 - l\right)^2$$

III. The Hamilton's equations of motion for this system are:

$$\begin{cases} \dfrac{\partial H\left(x_1, p_1, x_2, p_2; t\right)}{\partial p_1} = \dfrac{p_1}{m} = \dfrac{dx_1}{dt} \\[2mm] \dfrac{\partial H\left(x_1, p_1, x_2, p_2; t\right)}{\partial x_1} = -\dfrac{dp_1}{dt} \Rightarrow -K\left(x_2 - x_1 - l\right) = -\dfrac{dp_1}{dt} \\[2mm] \dfrac{\partial H\left(x_1, p_1, x_2, p_2; t\right)}{\partial p_2} = \dfrac{p_2}{m} = \dfrac{dx_2}{dt} \\[2mm] \dfrac{\partial H\left(x_1, p_1, x_2, p_2; t\right)}{\partial x_2} = -\dfrac{dp_2}{dt} \Rightarrow K\left(x_2 - x_1 - l\right) = -\dfrac{dp_2}{dt} \end{cases} \Rightarrow \begin{cases} \dfrac{dx_1}{dt} = \dfrac{p_1}{m} \\[2mm] \dfrac{dx_2}{dt} = \dfrac{p_2}{m} \\[2mm] \dfrac{dp_1}{dt} = K\left(x_2 - x_1 - l\right) \\[2mm] \dfrac{dp_2}{dt} = -K\left(x_2 - x_1 - l\right) \end{cases}$$

The Hamilton's equations yield the following equations of motion:

$$\frac{d^2 x_{1,2}}{dt^2} = \pm \frac{K}{m}(x_2 - x_1 - l)$$

These coupled first order equations can be solved by generating uncoupled second order equations (See Mathematica Notebook posted for this lecture).

$$\begin{cases} \dfrac{d^2}{dt^2}(x_1 + x_2) = 0 \\ \dfrac{d^2}{dt^2}(x_2 - x_1) = -\dfrac{2K}{m}(x_2 - x_1 - l) \end{cases} \Rightarrow \begin{cases} u = x_1 + x_2 \\ z = x_2 - x_1 - l \\ \dfrac{d^2 u}{dt^2} = 0 \\ \dfrac{d^2 z}{dt^2} + \dfrac{2K}{m}z = 0 \end{cases} \Rightarrow \begin{cases} x_1 = (u - z - l)/2 \\ x_2 = (u + z + l)/2 \\ u(t) = u(0) + \dfrac{du}{dt}\bigg|_{t=0} \cdot t \\ z(t) = Ae^{i\sqrt{2K/m}\cdot t} + Be^{-i\sqrt{2K/m}\cdot t} \end{cases}$$

If we take initial conditions to be $x_{1,2}(0) = \mp l$; $\dfrac{dx_{1,2}}{dt}\bigg|_{t=0} = 0$, then we find solutions:

$$x_{1,2} = \mp \frac{l}{2}\left(1 - \cos\sqrt{\frac{2K}{m}}t\right) = \mp l \sin^2 \sqrt{\frac{K}{2m}}t$$

Example IV: Longitudinal vibrations of a one 1D monoatomic lattice.
(Can also be applied to cubic crystals with a mono-atomic basis.)

    I. The system
Consists of ions located on a lattice defined by a lattice vector sa. The ions are assumed to be deviating from their respective lattice points by a distance u_s, which is taken to be smaller than the lattice constant a.
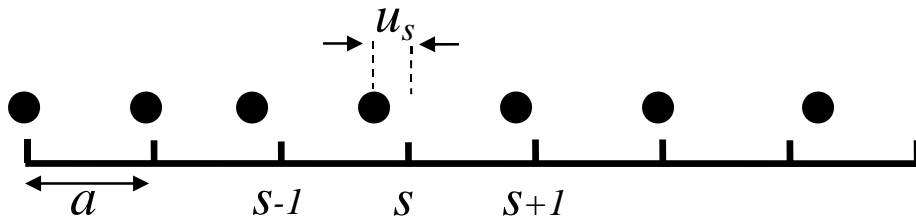
II. The Hamiltonian

We assume that the elastic energy is quadratic in the displacement, then we can write the total energy of the lattice is:

$$E^{lattice} = \sum_s \frac{mv_s^2}{2} + \sum_s K\frac{1}{2}(x_{s+1} - x_s - a)^2 = \sum_s \frac{p_s^2}{2m} + \sum_s \frac{K}{2}(u_{s+1} - u_s)^2$$

Then it is convenient to write a Hamiltonian for the crystal as a function of displacement u_s rather than coordinate x_s:

$$H = \sum_s \frac{p_s^2}{2m} + \frac{1}{2}K\sum_s \left(u_{s+1} - u_s\right)^2$$

III. Hamilton's equations of motion

Through the application of Hamilton's equations we derive the equations of motion:

$$\frac{\partial H}{\partial u_s} = -\frac{dp_s}{dt}$$

$$\frac{\partial H}{\partial p_s} = \frac{du_s}{dt}$$

Focus on the terms in the Hamiltonian that contain u_s and p_s

$$H_s = \frac{p_s^2}{2m} + \frac{1}{2}K\left(u_{s+1} - u_s\right)^2 + \frac{1}{2}K\left(u_s - u_{s-1}\right)^2 + \ldots +$$

We then obtain:

$$\frac{du_s}{dt} = \frac{p_s}{m}$$

$$\frac{dp_s}{dt} = K\left(u_{s+1} - u_s\right) - K\left(u_s - u_{s-1}\right) = K\left(u_{s+1} + u_{s-1} - 2u_s\right)$$

And the equations of motion are in the form: $\dfrac{d^2 u_s}{dt^2} = \dfrac{K}{m}\left(u_{s+1} + u_{s-1} - 2u_s\right)$

Look for solutions that have a time dependence of the form $\sim e^{-i\omega t}$, and substitute back in the above equation to obtain a *difference* equation:

$$u_s \propto e^{-i\omega t} \rightarrow \frac{d^2 u_s}{dt^2} = -\omega^2 u_s$$

$$\rightarrow -\omega^2 u_s = \frac{K}{m}\left(u_{s+1} + u_{s-1} - 2u_s\right)$$

This difference equation has solution of the form: $u_s = u_o e^{iksa}$, then $u_{s\pm1} = u e^{i(s\pm1)ka}$ where a is the lattice constant and k is called the wavevector (wavenumber as a scalar).
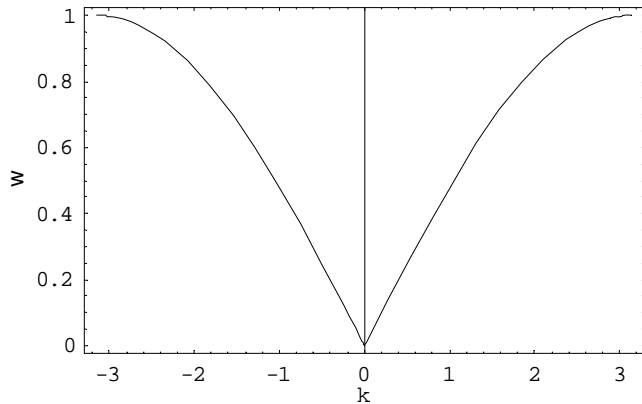
Then the total displacement of an ion *s* at time *t* can be written as: $u_k\left(s,t\right) = u_o e^{iksa - i\omega t}$
Substituting us into the difference equation above, we find:

$$-\omega^2 e^{iska} = \frac{K}{m}\left(e^{i(s+1)ka} + e^{i(s-1)ka} - 2e^{iska}\right) \Rightarrow -\omega^2 = \frac{K}{m}\left(e^{ika} + e^{-ika} - 2\right)$$

$$\Rightarrow \omega^2\left(k\right) = \frac{2K}{M}\left(1 - \cos ka\right) \Rightarrow \omega\left(k\right) = \sqrt{\frac{4K}{M}}\left|\sin \frac{ka}{2}\right|$$

Dispersion relations

The last equation defines the dispersion relation $\omega(k)$, which is a periodic function of **k**.

The dispersion relation constitutes a graphical representation of the independent solutions. If we know the boundary conditions, i.e. a vector of initial displacements $\left[u_1(0),...u_s(0),...\right]$ and initial velocities $\left[\left.\dfrac{du_1}{dt}\right|_{t=0},...\left.\dfrac{du_s}{dt}\right|_{t=0},...\right]$,

k and **ω** define a solution.

Physical characteristics of the solutions:

1. Crystal cannot transmit sound at frequencies above:

$$\omega_{max} = \sqrt{\frac{4K}{M}}$$

2. The ratio of two adjacent displacements is:

   $\dfrac{u_{s+1}}{u_s} = \dfrac{ue^{ik(s+1)a}}{ue^{iksa}} = e^{ika}$, which indicates that a solution involving k and a solution that has

   a k'=k+n2π/a are equivalent.

3. <u>Unique solutions</u> only for those values of k that are restricted to the first BZ: $-\dfrac{\pi}{a} \le k \le \dfrac{\pi}{a}$

4. <u>Phase velocity</u>: $c = \dfrac{\omega}{k}$ and <u>group velocity</u>: $v_g = \dfrac{d\omega}{dk} = \sqrt{\dfrac{Ka^2}{M}}\cos\dfrac{ka}{2}$
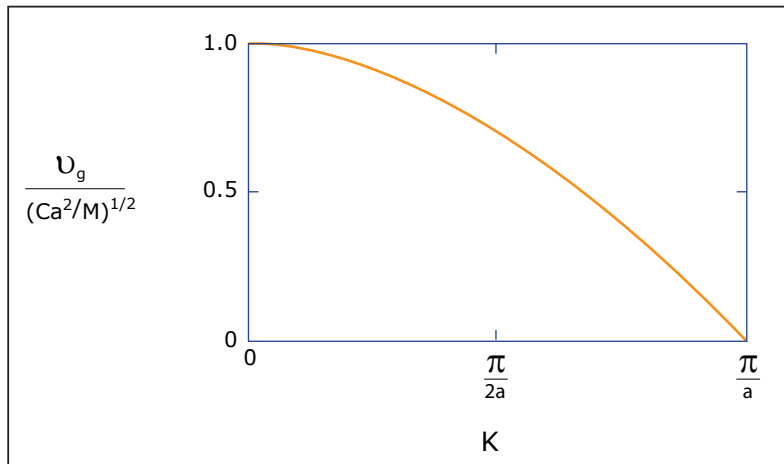

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5. <u>Standing waves</u> at the edge of the Brillouin zone for solutions where **k** satisfies: $k = \pm\dfrac{\pi}{a}$.

   Adjacent atoms move in opposite directions the wave is not propagating (group velocity is v_g=0).

This is the same condition that is satisfied when you get the so called Bragg reflections in optics (or x-ray diffraction). Recall the condition for Bragg diffraction:

$$2d\sin\theta = n\lambda; \quad \theta = \frac{\pi}{2}, \; d = a, \; \text{n=1} \rightarrow \lambda\text{=2a}$$

k is the wavevector and is related to the wavelength by: $k = \frac{2\pi}{\lambda} \Rightarrow k = \frac{2\pi}{2a} = \frac{\pi}{a}$

We just saw from the analysis above that we get standing waves at $k = \pm\frac{\pi}{a}$,

which is identical to the Bragg condition.

6. <u>Long wavelength limit</u> occurs when ka<<1. Under these conditions, the wavelength is much larger than the lattice spacing, chain can be treated as a continuum. The dispersion relations may be expanded in a Taylor series near ka=0:

$$\omega^2(k) = \frac{2K}{M}(1 - \cos ka)$$

$$\cos ka = 1 - \frac{(ka)^2}{2} + O\left((ka)^4\right)$$

$$\omega = \sqrt{\frac{K}{M}}ka$$

and the velocity of sound $v_g = \frac{d\omega}{dk} = \sqrt{\frac{K}{M}}a$ is independent of frequency, similar to the continuum model.

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